Some Considerations on the Additional Absorption Peak in the c-axis Infrared Conductivity of Bilayer Cuprate Superconductors: Interpretation of the Changes Induced by a Parallel Magnetic Field and the Role of Bilayer Splitting

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Changes of the $400\,\mathrm{cm}^{-1}$ peak in the c-axis conductivity of underdoped $YBa_2Cu_3O_{6.6}$ upon application of a parallel magnetic field reported by Kojima *et al.* are shown to be consistent with the model where the peak is due to the superfluid. Results of our calculations of the c-axis response of bilayer compounds with well defined bilayer-split bands are presented and discussed. For moderate values of the bilayer splitting ($\Delta\epsilon$ comparable to $2\Delta_{\max}$) the spectra of the superconducting state exhibit an additional mode which is due to the condensate and similar to the one of earlier phenonomenological approaches.

The c-axis infrared spectra of bilayer high-T_c cuprate superconductors (HTCS), i.e., HTC compounds with two CuO_2 planes within a unit cell, exhibit the following interesting features. At low temperatures a broad absorption peak develops in the spectra of the real part of the optical conductivity σ_1 in the frequency region between $300\,\mathrm{cm}^{-1}$ and $800\,\mathrm{cm}^{-1}$ (its frequency is material- and doping-dependent)[1,2,3,4,5]. At the same time some of the phonon modes are strongly renormalized, i.e., their frequencies and/or linewidths and/or spectral weights change[1,2,3,4]. The magnitude of the additional peak and the changes of the phonons are particularly spectacular for the strongly underdoped superconductor $YBa_2Cu_3O_{7-\delta}$ (Y-123)[3,6]. For a long time these phenomena had retained their mystery. In 2000 Grüninger *et al.*[7] showed that the additional peak in the spectra of Y-123 can be understood and quantitatively described in terms of a model proposed in 1996 by Van der Marel and Tsvetkov[8]. Within this model, the so called multilayer model, a bilayer compound is considered as a superlattice of homogeneously charged superconducting planes and interbilayer and intrabilayer regions as shown in Fig. 1.

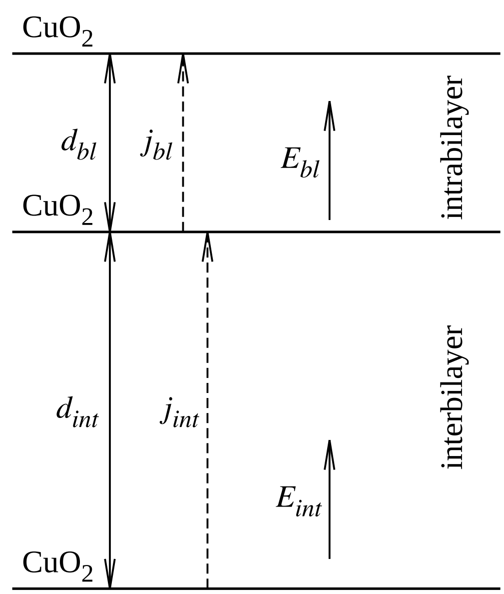

FIG. 1: Schematic representation of the multilayer model.

The model dielectric function $\varepsilon(\omega)$ is given by

$$\frac{d_{bl}+d_{int}}{\varepsilon(\omega)}=\frac{d_{bl}}{\varepsilon_{bl}(\omega)}+\frac{d_{int}}{\varepsilon_{int}(\omega)}\,, \tag{1}$$

$$\varepsilon_{bl/int}(\omega)=\varepsilon_{\infty}+\frac{i\sigma_{bl/int}(\omega)}{\varepsilon_0\omega}\,, \tag{2}$$

where ε_∞ is the interband dielectric constant and the conductivities σ_{bl} and σ_{int} are defined by $j_{bl}=\sigma_{bl}E_{bl}$ and $j_{int}=\sigma_{int}E_{int}$. In the superconducting state (SCS), they contain contributions of the condensate,

$$\sigma_{bl/int}(\omega)=\frac{i\varepsilon_0\omega^2_{bl/int}}{\omega}+\sigma^{reg}_{bl/int}(\omega)\,, \tag{3}$$

where ω_{bl} and ω_{int} are the plasma frequencies. Further σ^{reg}_{bl} and σ^{reg}_{int} are the regular parts of the conductivities. In the absence of the latter, $\varepsilon(\omega)$ exhibits two zero crossings, at $\omega_{L1}=\sqrt{\omega_{int}/\varepsilon_\infty}$ and at $\omega_{L2}=\sqrt{\omega_{bl}/\varepsilon_\infty}$, corresponding to two longitudinal plasma modes: the interbilayer and the intrabilayer one; in addition, it has a pole at

$$\omega_T=\sqrt{\frac{d_{bl}\omega^2_{int}+d_{int}\omega^2_{bl}}{(d_{bl}+d_{int})\varepsilon_\infty}} \tag{4}$$

corresponding to a so called transverse plasmon (TP). Its spectral weight is given by

$$S_T=\frac{\pi}{2}\varepsilon_0\frac{d_{bl}d_{int}(\omega^2_{bl}-\omega^2_{int})^2}{(d_{bl}+d_{int})(d_{bl}\omega^2_{int}+d_{int}\omega^2_{bl})}\,. \tag{5}$$

Grüninger *et al.* attributed the additional peak to the TP. The model has then been extended[6] by including local fields acting on the ions. This allowed the authors of Ref. 6 to explain not only the additional peak but

also the related phonon anomalies. Today, the multilayer model[8] and the local field idea[6] are becoming accepted. The nature of the intra-bilayer currents responsible for the additional peak, however, is the subject of an ongoing discussion[5,9]. Here we address two related issues.

Changes of the additional peak in strongly underdoped Y-123 induced by a parallel magnetic field have been studied by Kojima *et al.*[10]. It has been found that the field suppresses the condensate at $\omega = 0$. Its spectral weight (SW) is redistributed between a so called σ mode at ca $40\,\mathrm{cm}^{-1}$ and the additional peak at ca $400\,\mathrm{cm}^{-1}$. The SW increase of the latter amounts to ca $460\,\Omega^{-1}\mathrm{cm}^{-2}$. Surprisingly, the field does not influence the peak frequency. Below we show that this behaviour is consistent with the claim that the peak corresponds to the superconducting condensate. Assume for simplicity that the suppression of the superfluid in the interbilayer regions is complete, i.e., $\omega_{int} = 0$, that the field does not modify the intrabilayer plasma frequency ω_{bl} ($\omega_{bl} >> \omega_{int}$), and that the regular parts of the two conductivities can be neglected. The field induced changes of S_T and ω_T can then be obtained using Eq. (5) and Eq. (4), respectively,

$$\frac{\Delta S_T}{S_T} \approx \frac{(2d_{int} + d_{bl})}{d_{int}} \frac{\omega_{int}^2}{\omega_{bl}^2}\,, \tag{6}$$

$$\frac{\Delta \omega_T}{\omega_T} \approx -\frac{d_{bl}}{2d_{int}} \frac{\omega_{int}^2}{\omega_{bl}^2}\,. \tag{7}$$

It appears that S_T somewhat increases and ω_T very slightly decreases. For the values of the parameters obtained by fitting the spectra of a similarly underdoped Y-123 sample, $\omega_{bl} = 1200\,\mathrm{cm}^{-1}$, $\omega_{int} = 220\,\mathrm{cm}^{-1}$ (Ref. 6), $d_{bl} = 3.3$ Å and $d_{int} = 8.4$ Å, we obtain $\Delta S_T = 800\,\Omega^{-1}\mathrm{cm}^{-2}$ and $\Delta\omega_T = -3\,\mathrm{cm}^{-1}$. In reality, the suppression of the condensate in the interbilayer regions is certainly incomplete. Kojima and coworkers successfully interpreted the low-frequency part of the spectra in terms of a model where the Josephson coupling is considerably weakened only in ca 50% of the interbilayer regions. Using this model we obtain $\Delta S_T \approx 400\,\Omega^{-1}\mathrm{cm}^{-2}$ and $\Delta\omega_T \approx -1.5\,\mathrm{cm}^{-1}$ [the magnitudes are reduced ca by a factor of 0.5 with respect to the simple estimates of Eqs. (6) and (7)][11]. The value of ΔS_T is in excellent agreement with experiment. The very small value of $\Delta\omega_T$ accounts for the fact that, at first glance, the $400\,\mathrm{cm}^{-1}$ peak does not shift upon application of the field.

Transverse plasmon in the presence of bilayer splitting. The multilayer model of Eq. (1) is well justified[12] for a system of weakly ("Josephson") coupled CuO_2 planes where $t_{\perp\,\max}$ is much less than any important in-plane energy scale, in particular $t_{\perp\,\max} < \Delta_{\max}$. Here $t_{\perp\,\max}$ and $\Delta_{\max}$ are the maximum values of the interplanar hopping matrix element and the superconducting gap, respectively. The overdoped bilayer compound $Bi_2Sr_2CaCu_2O_8$ (Bi-2212), however, exhibits two bands: the bonding band (BB) and the antibonding band (AB), with the maximum splitting of ca 90 meV corresponding to $t_{\perp\,\max} = 45\,\mathrm{meV} > \Delta_{\max}$[13,14]. Here we present very preliminary results of our calculations of the c-axis response in such a system. Details will be presented in Ref. 15. The main ingredients of our approach are summarized below.

Our starting point is the tight-binding formalism outlined in Appendix B of Ref. 16 (with a more general form of the interplanar hopping matrix elements). For simplicity, the spacing layers will be supposed to be fully insulating (i.e., $t_{\perp\,int} = 0$ in the notation of Ref. 16). First, we express the intrabilayer conductivity $\sigma_{bl}(\omega)$ defined by $j_{bl}(\omega) = \sigma_{bl}(\omega)E_{bl}(\omega)$. It is given by Eq. (B9) of Ref. 16:

$$\sigma_{bl}(\omega) = \frac{[e^2 d_{bl}/(a^2\hbar^2)]\langle T\rangle + \chi(\mathbf{q}=0,\omega)}{i(\omega + i\delta)}\,, \tag{8}$$

where a is the in-plane lattice constant, T is the intrabilayer c-axis kinetic energy per unit cell,

$$\langle T\rangle = -\frac{2a^2}{(2\pi)^2}\int_{2D\,BZ} \mathrm{d}\mathbf{k}\, t_\perp(\mathbf{k})(n_{Bk} - n_{Ak})\,, \tag{9}$$

and χ is the relevant current-current correlation function,

$$\chi(\mathbf{q},\omega) = \frac{Na^2 d_{bl} i}{\hbar}\int_{-\infty}^{\infty} \mathrm{d}t \langle[j(\mathbf{q},t), j(-\mathbf{q},0)]\rangle \Theta(t) e^{i\omega t}\,. \tag{10}$$

The interplanar hopping matrix element $t_\perp$ is related to the dispersion relations of the two bands as $2t_\perp(\mathbf{k}) = \epsilon_{Ak} - \epsilon_{Bk}$. The occupation factors are denoted by n_{Bk} and n_{Ak}. In Eq. (10), $j(\mathbf{q},t)$ is the Fourier component of the paramagnetic part of the intrabilayer current density operator. It can be shown[15] that

$$j(\mathbf{q}=0) = \frac{ie}{Na^2\hbar}\sum_{\mathbf{K}=(\mathbf{k},k_z)} t_\perp(\mathbf{k})(c^+_{BK}c_{AK} - c^+_{AK}c_{BK})\,, \tag{11}$$

where c^+_{BK}, c_{BK}, c^+_{AK}, and c_{AK} are the conventional quasiparticle operators. The Matsubara counterpart $\chi(i\omega_m)$ of $\chi(\mathbf{q}=0,\omega)$ is given by[15]

$$\chi(i\omega_m) = \frac{4e^2 d_{bl}}{\hbar^3}\frac{1}{(2\pi)^2}\int \mathrm{d}\mathbf{k}\, t_\perp^2(\mathbf{k}) \times$$

$$\times \left\{ -\frac{1}{2\beta}\sum_{ip_n} \mathrm{Tr}\,[G_B(\mathbf{k}, ip_n) G_A(\mathbf{k}, ip_n + i\omega_m)] \right\}\,, \tag{12}$$

where G_B and G_A are the Nambu propagators. Note that for $G_B = G_A$ (i.e., in the limit of weak interlayer coupling) we recover Eq. (10) of Ref. 12. When deriving Eq. (12), vertex corrections have been neglected. In order to express the dielectric function, we have to consider interlayer Coulomb interactions. Random phase approximation leads to Eqs. (1), (2) with $\sigma_{int} = 0$. The multilayer formula (1) is thus justified even if the coupling between the closely-spaced planes is strong (the coupling across the spacing layer, however, must be negligible).

The results presented below have been obtained using the above equations with selfenergy corrections neglected. The final formula for χ reads

$$\chi(\omega) = \frac{e^2 d_{bl}}{\hbar^2(2\pi)^2}\int \mathrm{d}\mathbf{k}\, t_\perp^2(\mathbf{k})\times$$

$$\times\Big(l_1(\mathbf{k})[1-n_F(E_{Bk})-n_F(E_{Ak})]\times$$

$$\times\left\{\frac{1}{\hbar\omega+i\delta-E_k^+}-\frac{1}{\hbar\omega+i\delta+E_k^+}\right\}$$

$$+l_2(\mathbf{k})[n_F(E_{Ak})-n_F(E_{Bk})]\times$$

$$\times\left\{\frac{1}{\hbar\omega+i\delta-E_k^-}-\frac{1}{\hbar\omega+i\delta+E_k^-}\right\}\Big), \qquad (13)$$

where

$$l_{1/2}(\mathbf{k}) = \frac{\epsilon_{Bk}\epsilon_{Ak}+\Delta_{Bk}\Delta_{Ak}\mp E_{Bk}E_{Ak}}{E_{Bk}E_{Ak}}, \qquad (14)$$

$\Delta_{Bk/Ak}$ are the superconducting gaps, $E_{Bk/Ak} = \sqrt{\epsilon_{Bk/Ak}^2+\Delta_{Bk/Ak}^2}$, n_F is the Fermi function and $E_k^\pm = E_{Ak}\pm E_{Bk}$. A conventional form of the dispersion relations[17] has been used:

$$\epsilon_{B/A}(k) = -2t[\cos(k_x a)+\cos(k_y a)]-$$

$$4t'\cos(k_x a)\cos(k_y a)\mp\frac{t_{\perp\, max}}{4}[\cos(k_x a)-\cos(k_y a)]^2-\mu\,, \qquad (15)$$

and the bands have been assumed to possess the same superconducting gap

$$\Delta_{Bk} = \Delta_{Ak} = \frac{\Delta_{max}}{2}[\cos(k_x a)-\cos(k_y a)]\,. \qquad (16)$$

Figure 2 shows the main results
for the following values of the model parameters: $d_{bl} = 3.4$ Å, $d_{int} = 12.0$ Å (the values correspond to Bi-2212), $\varepsilon_\infty = 5.0$, $t = 250\,\mathrm{meV}$, $t' = -100\,\mathrm{meV}$, $t_{\perp\,\max} = 45\,\mathrm{meV}$[13], $\mu = -350\,\mathrm{meV}$, $\Delta_{\max} = 30\,\mathrm{meV}$, and $\delta = 1.0\,\mathrm{meV}$. In the normal state (NS, $\Delta_{\max} = 0$, $T = 100\,\mathrm{K}$), $\varepsilon_{bl\,2}(\omega)$ contains only the interband (IB) contribution. Its maximum is located at $\omega_{IB} \approx 2t_{\perp\,\max}/\hbar$. In the SCS ($T = 20\,\mathrm{K}$), $\varepsilon_{bl\,2}(\omega)$ consists of the IB (pair-breaking) contribution centered at $\omega_{IB} \approx 2\sqrt{t_{\perp\,\max}^2+\Delta_{\max}^2}/\hbar$, with a smaller SW than in the NS, and the one of the condensate (C) at zero frequency. The ratio SW(C)/SW(IB) depends on $\Delta_{\max}/t_{\perp\,\max}$. For $\Delta_{\max} = 20\mathrm{meV}$ (30meV; 60meV), e.g., we obtain $\omega_{bl} = 1870\,\mathrm{cm}^{-1}$, SW(C)/SW(IB) = 0.47 ($2260\,\mathrm{cm}^{-1}$, 0.93; $2690\,\mathrm{cm}^{-1}$, 3.07). The conductivity $\sigma_1(\omega)$ has sharp maxima labelled as P and Q (we do not consider here the small maximum labelled as Q'). They occur at frequencies ω_P and ω_Q, for which $\varepsilon_{bl\,1} = -(d_{bl}/d_{int})\varepsilon_\infty$ and $\varepsilon_{bl\,2}$ is small [see Eq. (1)]. The maximum Q has a large SW of about $60000\,\Omega^{-1}\mathrm{cm}^{-2}$. It appears already in the NS and it will be broadened by selfenergy effects. The large difference between ω_Q and ω_{IB} is caused by the interlayer Coulomb interactions. The maximum (mode) P appears only in the SCS as a result of broken gauge symmetry. Its frequency and SW (S_P) increase dramatically with increasing $\Delta_{\max}/t_{\perp\,\max}$. For $\Delta_{\max} = 20\mathrm{meV}$ (30meV; 60meV), e.g., we obtain $\omega_P = 350\,\mathrm{cm}^{-1}$, $S_P \approx 1300\,\Omega^{-1}\mathrm{cm}^{-2}$ ($490\,\mathrm{cm}^{-1}$, $2500\,\Omega^{-1}\mathrm{cm}^{-2}$; $840\,\mathrm{cm}^{-1}$, $13600\,\Omega^{-1}\mathrm{cm}^{-2}$). For $\Delta_{\max}/t_{\perp\,\max} \to 0$ (i.e., in the limit of strong interlayer coupling), the mode vanishes. Obviously, the maximum P can be related to the TP of the phenomenological model involving a superlattice of interbilayer and intrabilayer Josephson junctions. The underlying excitation can be visualized as a resonant oscillation of the condensate density between the closely-spaced CuO_2 planes.

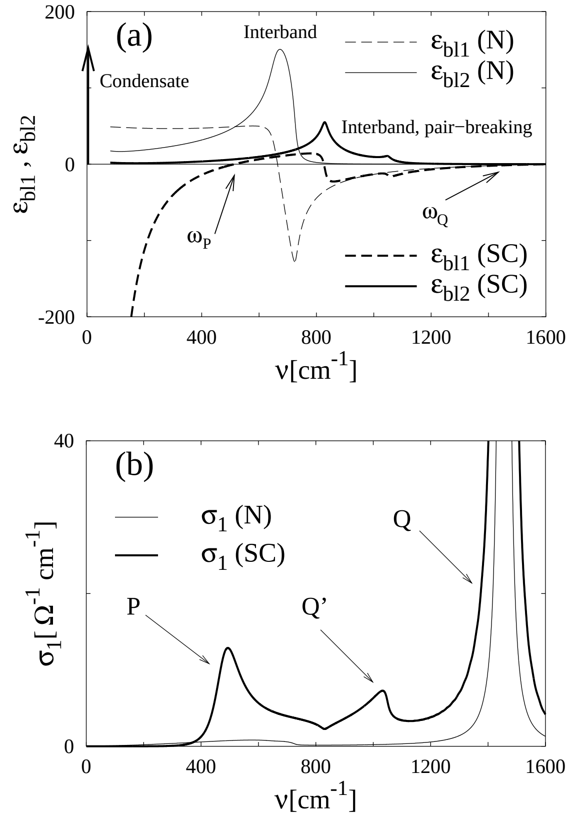

FIG. 2: Calculated spectra of the real (ε_{bl1}) and imaginary (ε_{bl2}) parts of the "intrabilayer dielectric function" ε_{bl} defined by Eq. (2) (a) and of the real part of the c-axis conductivity (b).

In conclusion, the changes of the $400\,\mathrm{cm}^{-1}$ peak induced by a parallel mg. field reported by Kojima *et al.* are consistent with the claim that it is related to the superconducting condensate. The regular parts of the two conductivities need not be taken into account in order to explain the changes. The c-axis response of bilayer compounds has been studied considering the B-A splitting. The conductivity σ_1 exhibits a maximum in MIR related to the B-A transitions. Its shape will be determined by selfenergy terms and it can be expected to change slightly when going from the NS to the SCS. *Only in the SCS*, an additional maximum appears in FIR, related to the condensate, with similar properties as the one of the naive Josephson-superlattice model. Our results indicate that the latter model is compatible with moderate values of the B-A splitting.

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